Claims

1. A computer for producing a three-dimensional representation of:

a. a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1; or

b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, wherein said computer comprises:

(i) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1;

(ii) a working memory for storing instructions for processing said computer-readable data;

(iii) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(iv) a display coupled to said central-processing unit for displaying said three-dimensional representation.

2. The computer according to claim 1, wherein the computer produces a three-dimensional representation of:

a. a molecule or molecular complex defined by structure coordinates of all of the human α-galactosidase amino acids set forth in FIG. 1, or

b. a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

wherein said computer readable data contains the coordinates of all of the human α-galactosidase amino acids set forth in FIG. 1.

3. A computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of human α-galactosidase according to FIG. 1;

(b) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex;

(c) a working memory for storing instructions for processing said computer-readable data of (a) and (b);

(d) a central-processing unit coupled to said working memory and to said computer-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said computer-readable data of (b) into structure coordinates; and

(e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.

4. The computer according to claim 3, wherein said molecule or molecular complex comprises a polypeptide having α-galactosidase activity.

5. A method for evaluating the potential of a chemical entity to associate with:

a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1, or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket defined by structure coordinates of human α-galactosidase amino acids W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å; and

ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

6. A method for identifying a potential agonist or antagonist of a molecule comprising a human α-galactosidase domain 1-like binding pocket comprising the steps of:

a. using the atomic coordinates of W47, D92, D93, Y134, C142, K168, D170, E203, L206, Y207, R227, D231, D266, and M267, according to FIG. 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a human α-galactosidase domain 1-like binding pocket;

b. employing said three-dimensional structure to design or select said potential agonist or antagonist;

c. synthesizing said agonist or antagonist; and

d. contacting said agonist or antagonist with said molecule to determine the ability of said potential agonist or antagonist to interact with said molecule.

7. The method according to claim 6, wherein in step a., the atomic coordinates of all the amino acids of human α-galactosidase according to FIG. 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å are used.